January 25, 2015

Dear EECE 503 students,

Here is my weekly letter to you (number 3) meant to help you find, arrange and summarize the material related to what was covered in class.

My first letter of January 15 reminded you where to find and master the introductory concepts related to topic 1 covered in: ChE 505 Ch.1N and ChE 505 Ch.2N. Together with topics covered in ChE 471: Lecture 1, 1A, 1B, 1C, 1D these represent the fundamentals for topics 1 and 2.

You may note that we did not cover in class ChE 505 Ch.2N Appendix. As long as you know how to find the number of independent reactions and solve equilibrium problems in systems with multiple reactions we do not need to go deeper into this topic at this stage. HW 2 should have helped you along these lines. We also did not yet cover in class ChE 505 Ch.3N on physical equilibria. We will do the key elements once we start to deal with multiphase systems. We will not address the specific jargon used in environmental engineering on equilibria in multiphase systems (the fundamentals are the same). The approach is outlined at the end of Chapter 3N. That is a starting point for consulting the literature on this topic.

In the previously distributed overall summary of key course concepts, which is posted on the web page below the Course Syllabus, the following three concepts topped the list of ten:
1. Stoichiometry, reaction progress, relationship to measures of composition, independent reactions.
2. Chemical and physical equilibria and equilibrium composition calculations.
3. Mechanisms and derivation of reaction rates.

The concepts below were covered last week (week 2):
Week 2. (Jan. 20, 22)
Concepts of kinetic rates, activation energy, elementary reactions, reaction mechanisms, derivation of rate forms from mechanisms by use of PSSA and RLSA. The difference between noncatalytic and catalytic reaction mechanisms. Chain reactions.
The topic of elementary reactions originally planned for Week 2 was moved to Week 3 which is now modified to read as follows:

In your teams, you should now prepare your own **TEAM SUMMARY ON CHEMICAL KINETICS and MECHANISMS** based on the material coved in class and in the notes related to the topics of Week 2 (See as example the summary I prepared for you on EECE 503 CHEMICAL EQUILIBRIUM CALCULATIONS – SUMMARY) and as a team submit to us in the same format the summary for week 2 by Monday, February 2 (Place a hard copy to Ms. Yu's pendaflex (Joyce's) in Brauer and send an electronic copy by e-mail to both of us). Submission is the responsibility of the team-leader for that week.

When summarizing kinetic rate of reaction, relationships between rates of various components, the meaning of the intrinsic rate of reaction, activation energy of reaction, power law dependence on composition, and ramifications of the choice of the driving force on activation energy value, you should read Ch. 4N up to p 15. Elementary reactions are introduced in Ch. 4N pp15-18. Starting from p18 on the section 5.4 on Combination and Disproportionation Gas Phase Reactions, to page 21 (on liquid reactions) is an important part to read after you read the chain reactions. **The principle of microscopic reversibility** is invoked to find the reverse rate of known elementary reactions and provides the link between kinetics and thermodynamics. Make sure that you do not miss that concept from the notes.

When summarizing mechanisms and derivation of rate forms from them, clarify the nature of catalytic reactions (closed sequence) and non-catalytic ones (open sequence). Explain PSSA and RLSA postulates; be cognizant of ozone homogeneous decomposition and catalytically induced one, Michealis Menten enzyme kinetics, chain reactions via free radical mechanism.

For these topics read carefully Ch. 5N up to p 14 section 5.4 on COMPARTMENTAL MODELING OF SINGLE PHASE SYSTEMS, Ch. 5N addendum and the section on Application of PSSA to Chain Reactions.

This should complete the summary for Week 2. Make up a problem or two to practice the key concepts.

The attached team HW3, due on Tuesday, February 3 may provide some inspiration for additional exercises.

During Week 3. (Jan. 27, 29) we plan to cover:
Transition state theory and elementary gas phase reactions (Ch. Section 6.2; section 6.4.1 electrolyte effect, pressure effect, chain reactions).

Transition state theory and elementary liquid phase reactions; solvent effects and electrostatic effects. Diffusion limited reactions. (Ch. 7N sections 7.4 pp4-6; 7.5 pp7-13; 7.8)

Compartmental models for single phase systems. Ch. 5 Sect. 5.4; pp 14-17.

Applications to ozone interactions with pollutants. (Ch. 5; sect.5.5 pp18-34)